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Higher order perturbation theory applied to radiative transfer in non-plane-parallel media

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Abstract

Radiative transfer in non-plane-parallel media is a very challenging problem, which is currently the subject of concerted efforts to develop computational techniques which may be used to tackle different tasks. In this paper we develop the full formalism for another technique, based on radiative perturbation theory. With this approach, one starts with a plane-parallel 'base model', for which many solution techniques exist, and treat the horizontal variability as a perturbation. We show that under the most logical assumption as to the base model, the first-order perturbation term is zero for domain-average radiation quantities, so that it is necessary to go to higher order terms. This requires the computation of the Green's function. While this task is by no means simple, once the various pieces have been assembled they may be re-used for any number of perturbations—that is, any horizontal variations.
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1. Introduction

Radiative perturbation theory [1], which derives from the mathematically related field of neutron transport theory [2], has proven to be an accurate and effective method of tackling radiative transfer problems over a period of 10 or more years [3–5]. In that time, it has been applied to a number of problems for which plane-parallel methods were appropriate [6–8]. In recent years, much attention has been turned to problems where such assumptions cannot be justified—the so-called 3D problems [9]. While there are a number of techniques available to tackle such problems [10–15], there is considerable interest both in developing new techniques, and in studying the inevitable trade-offs between computational intensity and the resulting accuracy [9]. We believe that perturbation theory

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can address many of these issues, and that it is capable of providing reasonable to good accuracy without placing excessive demands on computing resources.

In Section 2 we write the radiative transfer equation in operator notation, and introduce the adjoint transport operator. (Boundary conditions are addressed in the appendix). In Section 3 we introduce the Green's function, and show how the Dyson equation leads to a perturbation series for the radiative quantities of interest. Section 4 contains the material which is new: two specific applications involving media which are non-plane-parallel.

The first of these is the domain average of a quantity such as a surface or top-of-atmosphere flux. We show that, if we make logical assumptions as to the choice of base case, the first-order term is zero, so that it is necessary to derive the second and higher order terms. Thus we have no choice but to compute the Green's function. The second application is the high spatial resolution satellite observation. Here the first-order term is not zero. Efficient iteration schemes are presented to compute the full perturbation series in both cases.

2. Operator notation

The general (3D) scalar radiative transfer equation may be written as [2]

$$\vec{n}\cdot\vec{\nabla}I(\vec{r},\vec{n}) = -\sigma_{\rm e}(\vec{r})I(\vec{r},\vec{n}) + \sigma_{\rm s}(\vec{r})\int P(\vec{r},\vec{n}'\to\vec{n})I(\vec{r},\vec{n}')\,{\rm d}\vec{n}' + Q(\vec{r},\vec{n}). \tag{1}$$

Here $I(\vec{r},\vec{n})$ is the radiance at the point $\vec{r}$ in the direction $\vec{n}$, $\sigma_{\rm e}$ and $\sigma_{\rm s}$ are the extinction and scattering coefficients (or cross sections per unit volume), P is the phase function, and Q represents all sources of radiation, such as the solar beam coming in from the top of the atmosphere, a laser probe, or thermal emission. Note that we will generally interpret I as the total radiance field, both diffuse radiation and the direct beam (when present).

We now wish to write this equation in operator form, for future convenience:

$$\hat{L}I(\vec{r},\vec{n}') = Q(\vec{r},\vec{n}), \tag{2}$$

where the transport operator, $\hat{L}$, is clearly given by

$$\hat{L} \equiv \int {\rm d}\vec{n}'\{[\vec{n}'\cdot\vec{\nabla} + \sigma_{\rm e}(\vec{r})]\delta(\vec{n}-\vec{n}') - \sigma_{\rm s}(\vec{r})P(\vec{r},\vec{n}'\to\vec{n})\}\circ. \tag{3}$$

Note that the symbol $\circ$ is used to denote an integral operator, not a definite integral.

The transport operator is not self-adjoint, as it contains a first-order derivative, so we need to introduce the adjoint operator [2,3]. Consider a set of functions, $I(\vec{r},\vec{n})$, which obey certain boundary conditions, and a second set of functions, $\{\tilde{I}(\vec{r},\vec{n})\}$, which obey their own boundary conditions. For a given operator, $\hat{L}$, its adjoint, $\hat{\tilde{L}}$, is defined by, requiring that, for all $I(\vec{r},\vec{n})$ and $\tilde{I}(\vec{r},\vec{n})$

$$\langle\tilde{I},\hat{L}I\rangle = \langle\hat{\tilde{L}}\tilde{I},I\rangle, \tag{4}$$

where

$$\langle\phi_1,\phi_2\rangle \equiv \int {\rm d}\vec{r}\int {\rm d}\vec{n}\phi_1(\vec{r},\vec{n})\phi_2(\vec{r},\vec{n}) \tag{5}$$

denotes the 'inner product' of the indicated functions (or fields), as an integration over the 'phase space' variables of position and direction.

Note that throughout this work, we will interpret integration over our horizontal domain as an average value, that is

$$\int \mathrm{d}x \int \mathrm{d}y \equiv (XY)^{-1} \int_0^X \mathrm{d}x \int_0^Y \mathrm{d}y. \tag{5a}$$

The correct form of $\hat{\tilde{L}}$ will depend on the boundary conditions imposed on $\tilde{I}$ (and also on I, although this is assumed to have been set independently). Alternately, we may choose the form of the adjoint operator, and then determine what boundary conditions are required. Following Bell and Glasstone [2], we select the following adjoint operator:

$$\hat{\tilde{L}} \equiv \int \mathrm{d}\vec{n}' \{[-\vec{n}' \cdot \vec{\nabla} + \sigma_{\mathrm{e}}(\vec{r})]\delta(\vec{n}' - \vec{n}) - \sigma_{\mathrm{s}}(\vec{r})P(\vec{r}, \vec{n} \to \vec{n}')\} \circ \tag{6}$$

and leave questions of boundary conditions to the appendix. (Note that $\hat{\tilde{L}}$ can be derived from $\hat{L}$ by switching the two direction vectors, and changing the sign of the advection term. Physically we may regard this as a reversal of time of a photon's trajectory.)

We may now write the general adjoint transport equation in the form

$$\hat{\tilde{L}}\tilde{I}(\vec{r}, \vec{n}') = \tilde{Q}(\vec{r}, \vec{n}), \tag{7}$$

where $\tilde{Q}$ is a suitable (initially arbitrary) adjoint source.

2.1. Radiative effects

The purpose of solving the radiative transfer equation is to extract certain information from the (full) solution, I. Invariably this will consist of one or more numbers, such as the flux at the surface, heating rate in an atmospheric layer, or radiance measured by a suitably placed instrument looking in a certain direction. We refer to such specific pieces of information as radiative effects, E. Since all such information must be contained within I, it may be extracted using a suitable response function (or response operator), R, using the following functional relation [3]:

$$E = \langle R, I \rangle. \tag{8}$$

For example, the response function to obtain the vertical component of the net flux at the point $\vec{r}_0$ is clearly

$$R = \delta(\vec{r} - \vec{r}_0)\mu, \tag{9}$$

where we adopt the standard notation of 'μ' for the z-component of $\vec{n}$: the azimuth angle will be denoted by 'ϕ'.

While the standard way to obtain the value of the effect E is to solve the radiative transfer equation, and then apply Eq. (8), the adjoint formalism provides a second path. Consider the situation if we choose to use the response function, R, as the adjoint source in Eq. (7): the adjoint transport equation then becomes

$$\hat{\tilde{L}}\tilde{I} = R. \tag{10}$$

If we now take the inner product of this equation with I, and use the definition of the adjoint operator from Eq. (4), we obtain

$$\langle R, I\rangle = \langle \hat{\tilde{L}}\tilde{I}, I\rangle = \langle \tilde{I}, \hat{L}I\rangle = \langle \tilde{I}, Q\rangle. \tag{11}$$

Thus we see that we have two paths to our desired effect, E:

$$E = \langle R, I\rangle = \langle \tilde{I}, Q\rangle. \tag{12}$$

That is, we may start with the source, Q, solve the radiative transfer equation to obtain I, and then use R to extract the desired result. Alternately, we may start with the response function, R, solve the adjoint transport equation to obtain $\tilde{I}$, and use Q to extract the effect—essentially working backwards (although the radiative transfer equation, as we are using it, is not time dependent).

3. The Green's function

The Green's function for the operator $\hat{L}$ may be defined as the solution of the (transport) problem corresponding to a delta function source in both position and direction, that is [2,16]

$$\hat{L}G(\vec{r}, \vec{n}; \vec{r}_0, \vec{n}_0) = \delta(\vec{r} - \vec{r}_0)\delta(\vec{n} - \vec{n}_0). \tag{13}$$

(In the case of a plane-parallel problem, a suitably reduced Green's function may be defined.) The adjoint Green's function may be similarly defined via [2,16]

$$\hat{\tilde{L}}\tilde{G}(\vec{r}, \vec{n}; \vec{r}_0, \vec{n}_0) = \delta(\vec{r} - \vec{r}_0)\delta(\vec{n} - \vec{n}_0). \tag{14}$$

Since any source, Q, can be 'decomposed' as a (continuous) sum of delta functions, the radiance distribution for any source may be found from G using

$$I = \langle G, Q\rangle, \tag{15}$$

where the integrations are to be carried out over the second set of variables of G.

Similarly, we have

$$\tilde{I} = \langle \tilde{G}, R\rangle. \tag{16}$$

Note that it is often convenient to regard G and $\tilde{G}$ as operators (in fact, as the inverse transport operators—see below), and omit the angular brackets, as phase space integration will be implied. For example, Eq. (12) becomes

$$E = \langle R, GQ\rangle = \langle \tilde{G}R, Q\rangle. \tag{17}$$

This result is fully consistent with the above definition of the adjoint of an operator. This consistency may also be seen in the fundamental reciprocity relation between the Green's function and its adjoint [2]:

$$\tilde{G}(\vec{r}_1, \vec{n}_1; \vec{r}_2, \vec{n}_2) = G(\vec{r}_2, \vec{n}_2; \vec{r}_1, \vec{n}_1). \tag{18}$$

Note that the Green's function, and its adjoint, also obey the reciprocity relations:

$$G(\vec{r}_1, \vec{n}_1; \vec{r}_2, \vec{n}_2) = G(\vec{r}_2, -\vec{n}_2; \vec{r}_1, -\vec{n}_1); \tag{19a}$$

$$\tilde{G}(\vec{r}_1, \vec{n}_1; \vec{r}_2, \vec{n}_2) = \tilde{G}(\vec{r}_2, -\vec{n}_2; \vec{r}_1, -\vec{n}_1). \tag{19b}$$

In what follows, we will assume that G, and its adjoint, may be expanded in a double spherical harmonics series:

$$\tilde{G} = \sum_{n_1,k_1} \sum_{n_2,k_2} g_{n_1 n_2}^{k_1 k_2}(\vec{r}_1, \vec{r}_2) P_{n_1}^{k_1}(\mu_1) P_{n_2}^{k_2}(\mu_2) \cos k_1 \phi_1 \cos k_2 \phi_2. \tag{20}$$

Note that the limits to these summations will be set by computational considerations involving both accuracy requirements and resource constraints.

3.1. Dyson series

It is straightforward to show that G may be interpreted as the inverse transport operator to $\hat{L}$, and $\tilde{G}$ as the inverse operator to $\hat{\tilde{L}}$ [16]:

$$\hat{L}G = 1 = \hat{\tilde{L}}\tilde{G}, \tag{21}$$

where by '1' we mean an appropriate set of delta functions.

We have previously showed that G obeys a Dyson equation [16,17]

$$G = G_0 - G_0 \Delta\hat{L} G, \tag{22}$$

where G_0 is the Green's function for an operator $\hat{L}_0$, and G is the Green's function for the operator $\hat{L}$, where

$$\hat{L} = \hat{L}_0 + \Delta\hat{L}. \tag{23}$$

The spirit of the present work is that we assume that we have some atmospheric optical model, as defined by its transport operator, $\hat{L}_0$, for which we are able to solve the radiative transfer equation, and obtain G_0. Our aim is to obtain a suitable solution for the (presumably more complex) operator $\hat{L}$. This can be achieved if we first obtain G, which will always be possible if we are able to solve the Dyson equation. This is normally solved by successive substitution, leading to the series

$$G = G_0 - G_0\Delta\hat{L}G_0 + G_0\Delta\hat{L}G_0\Delta\hat{L}G_0 - G_0\Delta\hat{L}G_0\Delta\hat{L}G_0\Delta\hat{L}G_0\Delta\hat{L}G_0 \ldots \tag{24}$$

If this equation is now combined with Eq. (17) we obtain the perturbation series for E [16]:

$$E = E_0 - \langle \tilde{I}_0, \Delta\hat{L}I_0 \rangle + \langle \tilde{I}_0, \Delta\hat{L}G_0\Delta\hat{L}I_0 \rangle - \langle \tilde{I}_0, \Delta\hat{L}G_0\Delta\hat{L}G_0\Delta\hat{L}I_0 \rangle \ldots \tag{25}$$

4. Non-plane-parallel models

In previous work we have investigated the application of the higher order terms in Eq. (25) to plane-parallel model atmospheres [18–20], and we are currently undertaking further work in this area. However, it is in problems which are not plane-parallel where we see the most important applications of this formalism. There are many possible problems which fall under this heading, and in this paper we will consider just two. The first of these relates to situations where one is seeking the *domain average* of an azimuthally independent radiation quantity such as a flux in an atmospheric model which is not plane-parallel—for example a broken cloud field, or indeed a cloud layer with realistic internal heterogeneities. The second of these relates to the remote sensing of a cloud layer (for example) by a satellite with a high spatial resolution sensor—here it is the effect (and hence the response function, R) which is not plane-parallel, as well as the medium: see Section 4.2. Laser probing of cloud layers is essentially the adjoint of this problem. More complex situations may also be considered.

4.1. Domain-averaged fluxes

In climate modelling and numerical weather prediction, the models require the solar flux at the surface; for example, averaged over a (usually large) grid square. This is straightforward if the atmosphere above this square is plane-parallel, but less so if it is not, which is usually the case if (real) clouds are involved. In this case, both Q and R are plane-parallel (that is, they are independent of the horizontal coordinates, x and y). We therefore choose to start with a plane-parallel base model, corresponding to a plane-parallel transport operator, $\hat{L}_0$,

$$\hat{L}_0 = \int \mathrm{d}\vec{n}' \{[\vec{n}' \cdot \nabla + \sigma_{\mathrm{e}}^0(z)]\delta(\vec{n} - \vec{n}') - \sigma_{\mathrm{s}}^0(z) P^0(z, \vec{n}' \to \vec{n})\} \circ . \tag{26}$$

The full transport operator $\hat{L}$ will correspond to the actual atmospheric optical model. (Note that in a previous publication [1] it was erroneously assumed that $\hat{L}_0$ would only contain a derivative with respect to z, and that $\Delta\hat{L}$ would therefore contain derivatives with respect to x and y. This is incorrect: the transport operator *always* contains the three spatial derivatives. However, in plane-parallel situations the horizontal derivatives are redundant as nothing depends on these coordinates, by definition.)

In order to construct $\Delta\hat{L}$ in a suitable form, we need to expand the phase function in Legendre polynomials (assuming that the phase function depends only on the scattering angle)

$$\begin{aligned} P(\vec{r}, \vec{n}' \to \vec{n}) &= \sum_{\ell=0}^{N} (2\ell + 1)\chi_\ell(\vec{r}) P_\ell(\vec{n}' \cdot \vec{n})/4\pi \\ &= \sum_{\ell=0}^{N} \frac{(2\ell+1)}{4\pi} \chi_\ell(\vec{r}) \sum_{m=0}^{\ell} (2 - \delta_{0m}) \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(\mu) P_\ell^m(\mu') \cos m(\phi - \phi'). \end{aligned} \tag{27}$$

For convenience we further define

$$\eta_\ell(\vec{r}) \equiv \sigma_{\mathrm{s}}(\vec{r}) \chi_\ell(\vec{r}). \tag{28}$$

After expanding the phase functions in both transport operators in this fashion, it is straightforward to obtain the difference transport operator in the form

$$\begin{aligned} \Delta\hat{L} = \Delta\hat{\hat{L}} = \int \mathrm{d}\vec{n}' \Bigg\{ & \Delta\sigma_{\mathrm{e}}(\vec{r})\delta(\vec{n} - \vec{n}') - \sum_{\ell=0}^{N} \frac{(2\ell+1)}{4\pi} \\ & \times \Delta\eta_\ell(\vec{r}) \sum_{m=0}^{\ell} (2 - \delta_{0m}) \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(\mu) P_\ell^m(\mu') \cos m(\phi - \phi') \Bigg\} \circ . \end{aligned} \tag{29}$$

(Note that the difference operator is self-adjoint, as the derivative terms drop out.)

4.1.1. First-order term

Start by examining the first-order perturbation term, which we write using an obvious notation as

$$\Delta E_1 \equiv \langle \tilde{I}_0, \Delta L I_0 \rangle = \langle \Delta \hat{\tilde{L}} \tilde{I}_0, I_0 \rangle = \langle I_0, \Delta \hat{L} \tilde{I}_0 \rangle, \tag{30}$$

where we have used the definition of the adjoint operator, and the self-adjointness of $\Delta\hat{L}$. Since the effect we are seeking is, by assumption, azimuth independent, R will also be independent of ϕ', and so will the adjoint base case radiance, although the radiance need not be. We now let $\Delta\hat{L}$ operate on this adjoint radiance:

$$\Delta \hat{L} \tilde{I}_0 \equiv \int \mathrm{d}\vec{n}' \left\{ \Delta\sigma_{\mathrm{e}}(\vec{r})\delta(\vec{n} - \vec{n}')\tilde{I}_0(z, \mu') - \sum_{\ell=0}^{N} \frac{(2\ell+1)}{4\pi} \Delta\eta_\ell(\vec{r}) \right.$$

$$\left. \times \sum_{m=0}^{\ell} (2 - \delta_{0m}) \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(\mu) P_\ell^m(\mu') \cos m(\phi - \phi') \tilde{I}_0(z, \mu') \right\} \tag{31}$$

The integration over ϕ' is now trivial, and serves to reduce the summation over m to the $m = 0$ term only:

$$\Delta \hat{L} \tilde{I}_0 = \left\{ \Delta\sigma_{\mathrm{e}}(\vec{r}) \tilde{I}_0(z, \mu) - \int \mathrm{d}\mu' \sum_{\ell=0}^{N} \frac{(2\ell+1)}{4\pi} \Delta\eta_\ell(\vec{r}) 2\pi P_\ell(\mu) P_\ell(\mu') \tilde{I}_0(z, \mu') \right\}$$

$$= \left\{ \Delta\sigma_{\mathrm{e}}(\vec{r}) \tilde{I}_0(z, \mu) - \frac{1}{2} \sum_{\ell=0}^{N} (2\ell+1) \Delta\eta_\ell(\vec{r}) P_\ell(\mu) \tilde{\xi}_\ell(z) \right\}$$

$$= \frac{1}{2} \sum_{\ell} (2\ell+1) \{ \Delta\sigma_{\mathrm{e}}(\vec{r}) - \Delta\eta_\ell(\vec{r}) \} P_\ell(\mu) \tilde{\xi}_\ell(z), \tag{32}$$

where

$$\tilde{\xi}_\ell(z) \equiv \int \mathrm{d}\mu \, \tilde{I}_0(z, \mu) P_\ell(\mu). \tag{33}$$

The result of (32) is now a function of the spatial coordinates, and of μ. The base case radiance, I_0, will be a function of the spatial coordinates (in fact, only of z by definition of our base case), plus μ and ϕ (in general). We may now insert both of these quantities into Eq. (30) and perform the phase-space integrations to obtain

$$\Delta E_1 = \int \mathrm{d}\vec{r} \left\{ \Delta\sigma_{\mathrm{e}}(\vec{r}) \Xi(z) - \frac{1}{2} \sum_{\ell=0}^{N} (2\ell+1) \Delta\eta_\ell(\vec{r}) \xi_\ell(z) \tilde{\xi}_\ell(z) \right\}, \tag{34}$$

where

$$\xi_\ell(z) \equiv \int \mathrm{d}\mu \, I_0(z, \mu) P_\ell(\mu) \tag{35}$$

and

$$\Xi(z) \equiv \int \mathrm{d}\mu \, I_0(z, \mu) \tilde{I}_0(z, \mu). \tag{36}$$

Note that the three radiance ‘moments’ defined in Eqs. (33), (35) and (36) are independent of any perturbation, and thus need only be computed once.

We now note that, by our assumptions, the perturbation, as characterized by the parameters $\Delta\sigma_e$ and the $\Delta\eta_\ell$, is a function of the horizontal coordinates, whereas the radiance, adjoint radiance, and the above defined moments are not. We may thus perform the horizontal integrations, to arrive at

$$\Delta E_1 = 2\pi \int \mathrm{d}z \left\{ \Delta\bar{\sigma}_e(z)\Xi(z) - \frac{1}{2}\sum_{\ell=0}^{N}(2\ell+1)\Delta\bar{\eta}_\ell(z)\xi_\ell(z)\tilde{\xi}_\ell(z) \right\}, \tag{37}$$

where the overbar is used to denote the horizontal average of the quantities concerned.

We have now lost all information concerning the actual horizontal variations within our model atmosphere, and are left with just the average values. In fact, the most logical base model to take in applications such as this would be one with optical properties which are just the horizontal average of the actual medium. In this case, ΔE_1 vanishes identically.

4.1.2. Second-order term

We are left with no alternative but to turn to the second (and higher) order terms, which are much more difficult to compute because, of necessity, they contain the Green’s function. We will examine the second-order term in full detail, namely,

$$\Delta E_2 = \langle \tilde{I}_0, \Delta\hat{L}G_0\Delta\hat{L}I_0 \rangle = \langle I_0, \Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0 \rangle \tag{38}$$

using similar manipulations used before. By combining Eqs. (20) and (32) we obtain

$$\tilde{G}_0\Delta\hat{L}\tilde{I}_0 = \int \mathrm{d}\vec{r}_1 \int \mathrm{d}\mu_1 \int \mathrm{d}\phi_1 \sum_{n_2,k_2}\sum_{n_1,k_1} g_{n_2n_1}^{k_2k_1}(\vec{r}_2,\vec{r}_1)P_{n_2}^{k_2}(\mu_2)P_{n_1}^{k_1}(\mu_1)\cos k_2\phi_2 \cos k_1\phi_1$$
$$\times \left\{ \Delta\sigma_e(\vec{r}_1)\tilde{I}_0(z_1,\mu_1) - \frac{1}{2}\sum_\ell (2\ell+1)\Delta\eta_\ell(\vec{r}_1)P_\ell(\mu_1)\tilde{\xi}_\ell(z_1) \right\}. \tag{39}$$

The integral over ϕ_1 may now be done, eliminating the summation over k_1, and then the integral over μ_1 will eliminate the summation over ℓ. We then obtain

$$\tilde{G}_0\Delta\hat{L}\tilde{I}_0 = 2\pi \sum_{n_2,k_2} \Gamma_{n_2k_2}^{(2)}(\vec{r}_2)P_{n_2}^{k_2}(\mu_2)\cos k_2\phi_2, \tag{40}$$

where we define

$$\Gamma_{n_2k_2}^{(2)}(\vec{r}_2) \equiv \sum_{n_1}\int \mathrm{d}\vec{r}_1 g_{n_2n_1}^{k_20}(\vec{r}_2,\vec{r}_1)\{\Delta\sigma_e(\vec{r}_1) - \Delta\eta_{n_1}(\vec{r}_1)\}\tilde{\xi}_{n_1}(z_1). \tag{41}$$

We now need to operate on this result with the difference transport operator, $\Delta\hat{L}$:

$$\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0 = 2\pi \int \mathrm{d}\mu_2 \int \mathrm{d}\phi_2 \sum_{n_2,k_2} \Gamma_{n_2k_2}^{(2)}(\vec{r}_2)P_{n_2}^{k_2}(\mu_2)\cos k_2\phi_2 \left\{ \Delta\sigma_e(\vec{r}_2)\delta(\vec{n}_3-\vec{n}_2) \right.$$
$$\left. - \sum_\ell \frac{(2\ell+1)}{4\pi}\Delta\eta_\ell(\vec{r}_2)\sum_m (2-\delta_{0m})\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\mu_3)P_\ell^m(\mu_2)\cos m(\phi_3-\phi_2) \right\}. \tag{42}$$

Again we may perform the two angular integrations, in the process eliminating the summations over ℓ and m, finally obtaining

$$\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0 = 2\pi \sum_{n_2,k_2} \Gamma^{(3)}_{n_2k_2}(\vec{r}_2) P^{k_2}_{n_2}(\mu_3)\cos k_2\phi_3, \tag{43}$$

where we now define

$$\Gamma^{(3)}_{n_2k_2}(\vec{r}_2) \equiv \Gamma^{(2)}_{n_2k_2}(\vec{r}_2)\{\Delta\sigma_e(\vec{r}_2) - \Delta\eta_{n_2}(\vec{r}_2)\}. \tag{44}$$

(At this point, we will change the spatial label from $\vec{r}_2$ first to $\vec{r}$, and later to $\vec{r}_3$, for notational convenience.)

Finally we need to take the inner product of this expression with I_0, which we assume that we have also expanded in a spherical harmonics series,

$$I_0(z,\mu,\phi) \equiv \sum_{\ell,m} \frac{(\ell-m)!}{(\ell+m)!} I^m_\ell(z) P^m_\ell(\mu)\cos m\phi. \tag{45}$$

Hence

$$\langle I_0\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0\rangle = 2\pi \int \mathrm{d}r \int \mathrm{d}\mu \int \mathrm{d}\phi \sum_{\ell,m} \frac{(\ell-m)!}{(\ell+m)!} I^m_\ell(z) \sum_{n,k} \Gamma^{(3)}_{n,k}(\vec{r})$$
$$\times P^m_\ell(\mu) P^k_n(\mu)\cos m\phi \cos k\phi. \tag{46}$$

Again the angular integrations may be performed, eliminating the summations over ℓ and m, and finally yielding

$$\Delta E_2 = \langle I_0\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0\rangle = 2\pi^2 \int \mathrm{d}\vec{r} \sum_{n,k} I^k_n(z)\Gamma^{(3)}_{nk}(\vec{r}) \frac{2}{2n+1}(1+\delta_{0k}). \tag{47}$$

Note that the horizontal integration may be performed before the final step, as the radiance is independent of these variables.

4.1.3. Higher order terms

We may construct the third-order term

$$\Delta E_3 \equiv \langle I_0, \Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0\rangle \tag{48}$$

in an analogous manner to the previous term, and note that it leads to a relatively simple iteration scheme. We start with Eq. (43), and operate on it with Eq. (20):

$$\tilde{G}_0\Delta\hat{L}\tilde{G}_0\Delta\hat{L}\tilde{I}_0 = 2\pi \sum_{n_4,k_4}\sum_{n_3,k_3}\sum_{n_2,k_2} \int \mathrm{d}\vec{r}_3 g^{k_4k_3}_{n_4n_3}(\vec{r}_4,\vec{r}_3)\Gamma^{(3)}_{n_2k_2}(\vec{r}_3) P^{k_4}_{n_4}(\mu_4)\cos k_4\phi_4$$
$$\times \int \mathrm{d}\mu_3 \int \mathrm{d}\phi_3 P^{k_2}_{n_2}(\mu_3) P^{k_3}_{n_3}(\mu_3)\cos k_2\phi_2 \cos k_3\phi_3 \tag{49}$$
$$= 2\pi \sum_{n_4,k_4} \Gamma^{(4)}_{n_4k_4}(\vec{r}_4) P^{k_4}_{n_4}(\mu_4)\cos k_4\phi_4, \tag{50}$$

where

$$\Gamma^{(4)}_{n_4k_4}(\vec{r}_4) = \pi \sum_{n_3,k_3} (1+\delta_{k_30}) \frac{2}{2n_3+1} \frac{(n_3+k_3)!}{(n_3-k_3)!} \int \mathrm{d}\vec{r}_3 g^{k_4k_2}_{n_4n_3}(\vec{r}_4,\vec{r}_3)\Gamma^{(3)}_{n_3k_3}(\vec{r}_3). \tag{51}$$

Eq. (50) is now formally identical to Eq. (40), except that the dummy index 2 has become 4. Thus the remaining steps in the construction of the third-order term are identical to the corresponding terms in the construction of the second-order term, with all dummy indices increasing by 2. All higher order terms may be constructed in the same way. In practice, quantities such as Eq. (43) would be retained in computer memory before the final steps were carried out for a given order term, to act as the seed for the next order term. Iteration would thus be highly efficient.

Obtaining the Green's function in suitable form would still be a significant challenge for this technique. It needs to be remembered that it is the solution for a (general) point source within a plane-parallel medium (base case), and thus has most (but not all) of the complexity of the 3D problems we are addressing. Its prime simplification is that, due to the nature of the base case, it will possess translational symmetry:

$$G(\vec{r}_1,\vec{n}_1;\vec{r}_2,\vec{n}_2) = G(\vec{r}_1-\vec{\rho},\vec{n}_1;\vec{r}_2-\vec{\rho},\vec{\boldsymbol{n}}_{\boldsymbol{2}}), \tag{52}$$

where $\vec{\rho}$ is any vector in the two-dimensional (x,y) plane. The other key point to note is that the Green's function need only be computed a handful of times, for a set of suitably selected base cases (differing in optical thickness, for example), and then used in a wide variety of applications.

4.2. Local quantities

The second non-plane-parallel situation we wish to address occurs when we try to make local observations of radiation quantities in an inhomogeneous medium. (If the medium were plane parallel, this would clearly be a non-problem.) In these cases, either the source, Q, or the response function, R (or both), depend on the horizontal coordinates. Our base model will again be plane-parallel, but this time with optical properties identical to those in the column of the medium below the point where the observation is being made. (The other possibility is to take averaged properties for the base case, but over what spatial range should one average?)

4.2.1. Satellite observation

We consider this time the case of nadir viewing by a satellite with a high spatial resolution sensor; that is, it observes the upwelling radiance (intensity) from a small spot (x_o, y_o) at the 'top' of the medium $(z = z_{\mathrm{T}})$. Thus, the response function will be given by

$$R = \delta(\vec{r}-\vec{r}_o)\delta(\mu-1) \equiv \delta(x-x_o)\delta(y-y_o)\delta(z-z_{\mathrm{T}})\delta(\mu-1). \tag{53}$$

We start by examining the first-order term. From Eqs. (17), (24) and (15)

$$\Delta E_1 = \langle R, G_0\Delta\hat{L}G_0Q\rangle = \langle \Delta\hat{L}\tilde{G}_0R, G_0Q\rangle = \langle I_0, \Delta\hat{L}\tilde{G}_0R\rangle. \tag{54}$$

Starting from the right, we take the inner product of the adjoint Green's function with R, which immediately yields

$$\tilde{G}_0R = 2\pi \sum_{n,k} \Gamma^{(0)}_{nk}(\vec{r})P^k_n(\mu)\cos k\phi, \tag{55}$$

where we define

$$\Gamma^{(0)}_{nk}(\vec{r}) = (2\pi)^{-1} \sum_m g^{k0}_{nm}(\vec{r}, \vec{r}_o). \tag{56}$$

Eq. (55) is formally identical to Eq. (40). Thus, the remaining steps in obtaining this (first-order) term are exactly the same as the steps required to complete the second-order term in the domain average situation just considered. Note that, unlike that case, this time the first-order term is non-zero. Whether or not higher order terms will be required will depend on the degree of horizontal variability in the medium (especially close to the point of observation), and on the accuracy desired.

In an accompanying paper [21], we consider the case of a weak, sinusoidal horizontal perturbation in an otherwise plane parallel cloud, as has previously been examined by Li et al. using a non-adjoint perturbative technique [22,23]. The first-order term is computed using an extension of diffusion theory, and the results compared with a full simulation using SHDOM [14]. The essential features of the variability of the upwelling radiance are well captured with our approach.

4.2.2. Point fluxes

A problem very close to the previous is to ask for the vertical component of the net flux (upwelling flux) from a given point at the top of the medium (or downwelling flux at the bottom of the medium). In this case the response function becomes

$$R = \delta(\vec{r} - \vec{r}_o)\mu. \tag{57}$$

Taking the inner product with the adjoint Green's function yields essentially the same result, except that this time we have

$$\Gamma^{(0)}_{nk}(\vec{r}) = \tfrac{2}{3} g^{k0}_{n0}(\vec{r}, \vec{r}_o). \tag{58}$$

Again the remaining steps follow as before. Whether higher order terms are required will again depend on the (local) horizontal variability, and the desired accuracy.

It should be pointed out that the Green's function required in Eqs. (55) and (57) is a reduced version of the full Green's function, as its 'source' is the single point $\mathbf{r}_o$. Of course, if higher order terms are deemed necessary, the full Green's function will be required.

A number of applications of these results immediately spring to mind. Firstly, fluxes and flux divergences are the basis of local heating rates. In the case of non-plane-parallel media, it will, of course, be necessary to consider horizontal fluxes as well. These will be zero for the base model, of course, but not for the first-order perturbation term, provided that the base model is calculated based on the local optical properties, not the average properties.

A second application is to an examination of the models which are used to convert satellite intensity observations to fluxes, for Earth Radiation Budget-type studies. Here we would compare the effects of differing horizontal inhomogeneities on both Eqs. (56) and (58), and on the subsequent analysis to compute the first-order term in both these cases. Note that in both of these situations we do not need the full Green's function (although we would if higher order terms are required).

5. Discussion

There are a number of methods which have been proposed for solving horizontally inhomogeneous radiative transfer problems, and the choice of which one to implement will be strongly influenced by the nature of the problem under investigation. If high accuracy answers are required in specific geometries, then Monte Carlo [10] or SHDOM [14] are both suitable, provided sufficient computer time is available. However, if there are any changes to the optical properties of the medium—and the possibilities for such variations are endless—then the computations must start from scratch.

At the other extreme are techniques which are applicable to weak variability, such as will often be found in stratus clouds as a result of internal dynamical processes. The Independent Pixel Approximation [24] has been shown to have only limited applicability, so that a number of approximation techniques have recently been proposed. These include the non-adjoint perturbation approach of Li et al. [22,23], a Monte-Carlo-based approach [25], a diffusion approximation [26] and a modified Discrete Ordinate Method [27].

The approach presented in this paper falls somewhere between these extremes. It has the potential to achieve high accuracy, provided the computer resources are sufficient to compute the Green's function (this can certainly be done using a suitably modified version of SHDOM [14]). It also has the potential to be re-run for a wide range of cloud geometries and internal microphysics without major additional effort. As a consequence, one of its most obvious applications will be to study just which parameters, or parameter ranges, are likely to have greatest influence on particular radiation quantities. Even running our technique in a severely 'cut down' form—with minimal numbers of streams, for example—is likely to provide valuable insight into the most interesting regions of parameter space, which may then be more accurately explored using Monte Carlo or SHDOM.

One additional form of horizontal variability which we have not explicitly covered in the formalism of this paper concerns the surface reflection contribution. In a recent paper [28], Landgraf et al. have shown that the reflection characteristics of the lower boundary may be incorporated into the transport operator. As a consequence, they may also be treated as a perturbation within our formalism. Again, the base case would be for a horizontally uniform surface reflection function (not necessarily Lambertian), with the perturbed model incorporating the true surface variability. We will explore these possibilities in the near future.

Appendix A. Boundary conditions

The adjoint of an operator, and its corresponding boundary conditions, are intimately related. In some problems, adjoint boundary conditions may be imposed first, and the corresponding adjoint operator derived using Eq. (4). In other problems, the reverse procedure is more appropriate. Experience and mathematical intuition are often the best guides to the most appropriate path to take. The 'standard' approach in dealing with operators containing first-order derivatives is to swap the sign of this term, as in Eq. (6), and then use integration by parts to determine the boundary conditions.

Upon substituting both Eqs. (3) and (6) into (4), all terms but the derivatives immediately cancel, leaving

$$\langle \tilde{I}, LI \rangle - \langle \tilde{L}\tilde{I}, I \rangle = \int\int \{ \tilde{I}(\vec{n} \cdot \nabla I) + (\vec{n} \cdot \nabla \tilde{I}) I \} \, \mathrm{d}\vec{r} \, \mathrm{d}\vec{n}. \tag{A.1}$$

Now, since ∇ does not operate on directions, we may write

$$\vec{n} \cdot \nabla I = \nabla \cdot (\vec{n} I)$$

and similarly for $\tilde{I}$. By noting the chain rule, we thus obtain

$$\langle \tilde{I}, LI \rangle - \langle \tilde{L}\tilde{I}, I \rangle = \int \int \nabla \cdot (\vec{n} I \tilde{I}))\, \mathrm{d}\vec{r}\, \mathrm{d}\vec{n}. \tag{A.2}$$

This volume integral may be converted to a surface integral using the divergence theorem (essentially a three-dimensional integration by parts):

$$\langle \tilde{I}, LI \rangle - \langle \tilde{L}\tilde{I}, I \rangle = \int \int \hat{\mathbf{n}} \cdot \vec{n} I \tilde{I}\, \mathrm{d}A\, \mathrm{d}\vec{n}, \tag{A.3}$$

where $\hat{\mathbf{n}}$ is the out-going unit normal. We require, of course, that this quantity be zero. In nuclear reactor theory, this is achieved by noting that as there are no incoming neutrons (photons), half of the surface integral is automatically zero. If we now require that there be no outgoing adjoint neutrons (photons), the other half will also be zero. That is, our twin boundary conditions, one physical, and one mathematical, are that, on the boundary of the medium

$$I(\vec{r}, \vec{n}) = 0 \quad \text{for } \hat{\mathbf{n}} \cdot \vec{n} < 0 \tag{A.4a}$$

and

$$\tilde{I}(\vec{r}, \vec{n}) = 0 \quad \text{for } \hat{\mathbf{n}} \cdot \vec{n} > 0. \tag{A.4b}$$

This solution is not available to us in this situation, however, as our medium does not have identifiable boundaries in the horizontal directions. We do have clearly defined boundaries at the top and bottom of our medium of course, and may therefore impose Eqs. (A.4) on those, as has previously been done in the plane-parallel case. In the horizontal, our medium extends indefinitely, although we prefer not to say 'to infinity'. In order to numerically compute the Green's function, it will clearly be necessary to restrict our attention to finite media, which raises its own concerns, independent of adjoint boundary conditions. Nevertheless, any solution must address both issues. We believe that the most logical approach is to consider a rectangular domain, and to impose periodic boundary conditions on both the intensity, and adjoint intensity functions. That is, whatever leaves through one boundary face must reenter the medium through the opposite face.

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